SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name:	Number 30 5-02/	Z Serial Nur	nber: <u>1005</u> 2	22.96	*	·
If more than one search is subm	itted, please prioriti	ze searches in c	order of need.			•
Please provide a detailed statement of the Include the elected species or structures, k utility of the invention. Define any terms known. Please attach a copy of the cover s	search topic, and describe eywords, synonyms, acroi that may have a special m	nyms, and registry no eaning. Give examp	umbers, and combin	e with the concept or	**** 	
Title of Invention:	. In ox	· Latine	Coloration	et bais		
Inventors (please provide full names):	15 tar 0x	m et al.	-	·	_	
Earliest Priority Filing Date: *For Sequence Searches Only* Please include appropriate serial number.	1/23 / 700) le all pertinent information (al, or issued patent n	umbers) along with the		
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STAFF USE ONLY	Type of Search	<i>"</i> ,	and cost where ap	plicable		•
Searcher: 9, Full	NA Sequence (#)	STN				
Searcher Phone #:Searcher Location:	Structure (#)	Dialog				
Date Searcher Picked Up:	Bibliographic	Questel/Orbit Dr.Link				
Date Completed: 8/14/03	Litigation	Lexis/Nexis				•
Searcher Prep & Review Time: 20	Fulltext	Sequence Systems				
Clerical Prep Time:	Patent Family	WWW/Internet				e de la companya de l
Online Time:	Other	Other (specify)		BES	T AVAIL	WILL UUT

ELHILO 10/052296 8/14/03 Page 1

=> FILE REG

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STRUCTURE FILE UPDATES: 13 AUG 2003 HIGHEST RN 566135-25-9 DICTIONARY FILE UPDATES: 13 AUG 2003 HIGHEST RN 566135-25-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

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Crossover limits have been increased. See HELP CROSSOVER for details.

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=> FILE HCAPLUS

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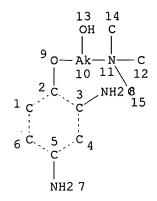
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FILE COVERS 1907 - 14 Aug 2003 VOL 139 ISS 7 FILE LAST UPDATED: 13 Aug 2003 (20030813/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> D OUE

L4 STR



16 structures from this query

NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

16 SEA FILE=REGISTRY SSS FUL L4 L7 2 SEA FILE=HCAPLUS ABB=ON L6

L82 SEA FILE=HCAPLUS ABB=ON L7 AND (HAIR OR KERAT?)

=> D L8 ALL HITSTR 1-2

references

ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2003 ACS on STN 2002:574892 HCAPLUS ANDN 137:129544 applicant

8/14/03

Couplers for oxidative coloration of hair ΤI

ΙN Lim, Mu-Ill; Pan, Yuh-Guo; Anderson, James S.

PA Clairol Incorporated, USA

PCT Int. Appl., 49 pp. SO CODEN: PIXXD2

Patent DT

English LΑ

ICM A61K007-13 IC

CC 62-3 (Essential Oils and Cosmetics)

PATENT NO. KIND DATE APPLICATION NO. WO 2002058659 A1 20020801 WO 2002-US1636 20020118 PΙ W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG US 2002144700 A1 20021010 US 2002-52296

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20010123
PRAI US 2001-263551P
    MARPAT 137:129544
OS
     Couplers for hair coloring compns. for oxidative dyeing of
AB
    hair are [3-(2,4-diaminophenoxy)-2-hydroxypropyl]trialkylammonium
     halides or sulfates. For example, a hair dye was formulated
     contg. [3-(2,4-diaminophenoxy)-2-hydroxypropyl]trimethylammonium bromide,
     p-toluenediamine (as primary dye intermediate), and conventional
    hair prepn. ingredients.
ST
    hair dye coupler quaternary ammonium compd
    Hair preparations
IT
        (dyes; hair dyes contg. couplers and oxidn. dye primary
        intermediates)
     90-15-3, Naphthalen-1-ol 95-55-6, 2-Aminophenol
IT
                                   95-88-5, 4-Chlorobenzene-1,3-diol
     2-Methylbenzene-1,4-diamine
     106-50-3, Benzene-1, 4-diamine, biological studies
                                                         108-46-3,
     Benzene-1,3-diol, biological studies
                                          123-30-8, 4-Aminophenol
                           591-27-5, 3-Aminophenol
                                                    608-25-3,
     4-Methylaminophenol
     2-Methylbenzene-1,3-diol
                                1004-74-6, Pyrimidinetetramine
                    2835-95-2, 5-Amino-2-methylphenol
                                                         2835-98-5,
     1H-Indol-6-ol
                             2835-99-6, 4-Amino-3-methylphenol
     2-Amino-5-methylphenol
     2-Methyl-naphthalen-1-ol 7575-35-1
                                            16867-03-1, 2-Aminopyridin-3-ol
     17672-22-9, 2-Amino-6-methylphenol 26021-57-8, 3,4-Dihydro-2H-1,4-
     benzoxazin-6-ol 41927-22-4, 4-Methyl-2-phenyl-2,4-dihydro-3H-pyrazol3-
           53222-92-7, 3-Amino-2-methylphenol
                                                55302-96-0,
     5-(2-Hydroxyethylamino)2-methylphenol
                                            70643-19-5, 2-(2,4-
     Diaminophenoxy) ethanol
                              83763-47-7
                                          93841-24-8, 2-(2,5-
     Diaminophenyl) ethanol
                             94082-77-6
                                          129697-50-3 131311-66-5
     155601-17-5
                  157469-54-0
                                 220264-60-8
                                               307493-94-3,
     3-(2,4-Diaminophenoxy)propan-1-ol
                                         329320-36-7
     RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
        (hair dyes contg. couplers and oxidn. dye primary
        intermediates)_
IT
     444155-06-0 444155-07-1 444155-09-3
     444155-10-6 444155-12-8 444155-13-9
     444155-14-0 444155-15-1 444155-16-2
     444155-18-4 444155-20-8
     RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
        (novel couplers for oxidative hair dyes)
ΙT
     19652-60-9P
     RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of hair dye couplers)
ΙT
     51-28-5, 2,4-Dinitrophenol, reactions
                                             535-80-8, m-Chlorobenzoic acid
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (prepn. of hair dye couplers)
TT
     10242-18-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of hair dye couplers)
RE.CNT 2
             THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Bugaut; DE 3302534 A1 1983 HCAPLUS
(2) Rose; DE 2948093 Al 1981 HCAPLUS
IΤ
     444155-06-0 444155-07-1 444155-09-3
     444155-10-6 444155-12-8 444155-13-9
     444155-14-0 444155-15-1 444155-16-2
     444155-18-4 444155-20-8
     RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
```

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10/052296

8/14/03

Page 4

(novel couplers for oxidative hair dyes)

RN 444155-06-0 HCAPLUS

CN 1-Propanaminium, 3-(2,4-diaminophenoxy)-2-hydroxy-N,N,N-trimethyl-, bromide (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NH}_2 \\ \text{O-CH}_2\text{-CH-CH}_2\text{-N+Me}_3 \\ \\ \text{H}_2\text{N} \end{array}$$

• Br-

RN 444155-07-1 HCAPLUS

CN 1-Propanaminium, 3-(2,4-diaminophenoxy)-N,N,N-triethyl-2-hydroxy-, chloride (9CI) (CA INDEX NAME)

● c1-

RN 444155-09-3 HCAPLUS

CN 1-Propanaminium, 3-(2,4-diaminophenoxy)-2-hydroxy-N,N,N-tripropyl-, propyl sulfate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 444155-08-2 CMF C18 H34 N3 O2

$$NH_2$$
 OH $O-CH_2-CH-CH_2-N^+(Pr-n)_3$

CM 2

ELHILO

10/052296

8/14/03

Page 5

CRN 72640-73-4

CMF C3 H7 O4 S

n-Pr-0-S03-

RN 444155-10-6 HCAPLUS

CN 1-Propanaminium, 3-(2,4-diaminophenoxy)-2-hydroxy-N,N,N-tris(2-hydroxyethyl)-, bromide (9CI) (CA INDEX NAME)

• Br-

RN 444155-12-8 HCAPLUS

CN 1-Propanaminium, 3-(2,4-diaminophenoxy)-2-hydroxy-N,N-bis(2-hydroxyethyl)-N-methyl-, methyl sulfate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 444155-11-7 CMF C14 H26 N3 O4

CM 2

CRN 21228-90-0 CMF C H3 O4 S

Me- 0- SO3-

RN 444155-13-9 HCAPLUS

CN 1-Propanaminium, 3-(2,4-diaminophenoxy)-2-hydroxy-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)

ELHILO 10/052296

8/14/03

Page 6

● c1-

RN 444155-14-0 HCAPLUS

CN 1-Propanaminium, 3-(2,4-diaminophenoxy)-N,N,N-triethyl-2-hydroxy-, bromide (9CI) (CA INDEX NAME)

● Br-

RN 444155-15-1 HCAPLUS

CN 1-Propanaminium, 3-(2,4-diaminophenoxy)-2-hydroxy-N,N,N-tripropyl-, bromide (9CI) (CA INDEX NAME)

● Br-

RN 444155-16-2 HCAPLUS

CN 1-Propanaminium, 3-(2,4-diaminophenoxy)-2-hydroxy-N,N,N-tripropyl-, chloride (9CI) (CA INDEX NAME)

$$NH_2$$
 OH $O-CH_2-CH-CH_2-N+(Pr-n)_3$

● cl -

RN 444155-18-4 HCAPLUS

CN 1-Propanaminium, 3-(2,4-diaminophenoxy)-2-hydroxy-N,N,N-trimethyl-, methyl sulfate (salt) (9CI) (CA INDEX NAME)

CM 1

ELHILO

CRN 444155-17-3 CMF C12 H22 N3 O2

$$^{\rm NH_2}$$
 $^{\rm OH}$ $^{\rm OH}$ $^{\rm CH_2-CH-CH_2-N+Me_3}$ $^{\rm H_2N}$

CM 2

CRN 21228-90-0 CMF C H3 O4 S

Me- 0- SO3-

RN 444155-20-8 HCAPLUS

CN 1-Propanaminium, 3-(2,4-diaminophenoxy)-N,N,N-triethyl-2-hydroxy-, ethyl sulfate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 444155-19-5 CMF C15 H28 N3 O2

CM 2

CRN .48028-76-8 CMF C2 H5 O4 S

Et- 0- SO3-

L8 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2003 ACS on STN

AN 1983:577512 HCAPLUS

DN 99:177512

TI Amino compounds useful as hair dyes

IN Bugaut, Andree; Genet, Alain

PA Oreal S. A., Fr.

SO Ger. Offen., 93 pp.

CODEN: GWXXBX

DT Patent

LA German

IC C07C093-14; A61K007-13

CC 41-8 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)

Section cross-reference(s): 62

FAN.CNT 1

FAN.	CNT	1						
	PATENT NO.		KIND	DATE	AP	PLICATION NO.	DATE	
ΡI	DE	3302534	A1	19830804	DE	1983-3302534	19830126	
	CH	661501	Α	19870731	CH	1983-273	19830118	
•	FR	2520358	A1	19830729	FR	1983-847	19830120	
	FR	2520358	В1	19850524				
	CA	1191849	A1	19850813	CA	1983-420080	19830124	
	ΑT	8300220	Α	19880515	AT	1983-220	19830124	
	ΑT	387212	В	19881227				
	BE	895697	A1	19830725	BE	1983-209961	19830125	
	ΑU	8310762	A1	19830804	AU	1983-10762	19830125	
	ΑU	556627	B2	19861113				
	GB	2113685	·Al	19830810	GB	1983-1981	19830125	
	GB	2113685	B2	19851211		•		
	NL	8300267	Α	19830816	NL	1983-267	19830125	
	ES	519237	A1	19840716	ES	1983-519237	19830125	
	JР	58164553	A2	19830929	JP	1983-10007	19830126	
	GB	2129022	A1	19840510	GB	1983-31092	19831122	
	GB	2129022	B2	19851211				
	US	4888025	Α	19891219	US	1985-742240	19850607	
	ΑU	8666832	A1	19870416	AU	1986-66832	19861222	
PRAI	LU	1982-83900		19820126				
	LU	1982-84391		19820927				

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US 1983-459964 19830121 GB 1983-1981 19830125

I

GI

3-Amino-1-(substituted phenoxy)-2-propanols (I; R = NO2, NH2; R1 = NH2, AΒ C1-4 alkyl- or hydroxyalkyl-substituted amino, morpholino, piperidino, quaternary ammonium; R2, R3 = H, C1-4 alkyl or hydroxyalkyl) are prepd. and used in hair dyeing formulations. Depending on the nature of R and its position with respect to NR2R3, I can be used as direct dyes (R = NO2) or (R = NH2) as oxidn. bases or couplers. Thus, reaction of 4,3-AcNH(O2N)C6H3OH [7403-75-0] with epichlorohydrin to form the glycidyl ether (II) [24544-37-4], treatment of II with Et2NH to give 4,3-AcNH(O2N)C6H3OCH2CH(OH)CH2NEt2 (III) [87563-65-3], and deacetylation of III gave 4,3-H2N(O2N)C6H3OCH2CH(OH)CH2NEt2.HCl [87563-64-2], a direct dye. Hydrogenation of 2,4-H2N(O2N)C6H3OCH2CH(OH)CH2NMe2 [87563-66-4], followed by N-acetylation, quaternization with MeI, and deacetylation gave 2,4-(H2N)2C6H3OCH2CH(OH)CH2N+Me3Cl-.2HCl [87570-61-4], a coupler for oxidative dyeing compns. Nine other I were prepd. by these and similar methods, and dyeing formulations contg. these dyes are described in detail.

aminophenoxypropanol hair dye; phenylenediamine deriv hair dye; nitroaminophenol ether hair dye; coupler oxidative hair dye; oxidn base hair dye

IT Alcohols, uses and miscellaneous

RL: USES (Uses)

(amino, for direct and oxidative hair dyes)

IT Hair preparations

(dyes, direct, aminophenoxypropanol derivs. as)

IT Hair preparations

(dyes, oxidative, aminophenoxypropanol derivs. as bases and couplers for)

IT 80062-31-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(epoxidn. of, by cyclodehydration) .

IT 97-60-9 7403-75-0 25351-89-7

RL: RCT (Reactant); RACT (Reactant or reagent) (etherification of, by epichlorohydrin)

IT 87563-58-4

RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrogenation of)

IT 87563-48-2P 87563-50-6P 87570-61-4P

RL: IMF (Industrial manufacture); PREP (Preparation)

(manuf. and use of, as coupler for oxidative hair dyeing

compns.)

IT 87563-42-6P 87563-43-7P 87563-44-8P 87563-45-9P 87563-46-0P 87563-49-3P 87563-64-2P

RL: IMF (Industrial manufacture); PREP (Preparation) (manuf. and use of, as direct dye for hair) IT 87563-47-1P RL: IMF (Industrial manufacture); PREP (Preparation) (manuf. and use of, as oxidn. base for hair dyeing compns.) IT 87563-51-7P 87563-52-8P 87563-56-2P 87563-61-9P 87563-63-1P 87563-65-3P 87570-60-3P RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (prepn. and deacetylation of) ΙT 87563-66-4P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and hydrogenation of) ΙT 87563-53-9P 87563-55-1P 87563-60-8P RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (prepn. and hydrolysis of) IT . 87563-62-0P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and quaternization of) ΙT 24544-37-4P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and reaction of, with amines) IT 78917-60-9P 87563-54-0P 87563-59-5P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and reaction of, with succinimide) ΙT 87563-57-3P RL: IMF (Industrial_manufacture); PREP-(Preparation)-(prepn. of) IT 87570-61-4P RL: IMF (Industrial manufacture); PREP (Preparation) (manuf. and use of, as coupler for oxidative hair dyeing compns.) RN 87570-61-4 HCAPLUS

1-Propanaminium, 3-(2,4-diaminophenoxy)-2-hydroxy-N,N,N-trimethyl-,

chloride, dihydrochloride (9CI) (CA INDEX NAME)

$$O-CH_2-CH-CH_2-N+Me_3$$

CN

C1 -

2 HCl

ELHILO